The Chemistry Maths Book

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Solutions

Chapter 20 Numerical methods

Section 20.2

1. Express the following numbers rounded to (a) 3 decimal places, (b) 4 significant figures:

(i) 1.21271 → (a) 1.213 (b) 1.213

(ii) 72.0304 → (a) 72.030 (b) 72.03

(iii) 0.129914 → (a) 0.130 (b) 0.1299

(iv) 0.0024988 → (a) 0.002 (b) 0.002499

2. Find the absolute error bound for each answer of Exercise 1.

(i) (a) 0.0005 (b) 0.0005

(ii) (a) 0.0005 (b) 0.005

(iii) (a) 0.0005 (b) 0.00005

(iv) (a) 0.0005 (b) 0.0000005

3. Compute the values of the following arithmetic expressions. Assuming that all the numbers in the expressions are correctly rounded, find the absolute error bounds of your answers:

(i) $2.137+3.152 \rightarrow (2.137\pm 0.0005)+(3.152\pm 0.0005)=6.289\pm 0.001$

(ii) $2.137+3.152-4.672 \rightarrow (6.289\pm 0.001)-(4.672\pm 0.0005)=1.617\pm 0.0015$

(iii) $12.36+14.13+16.38 \rightarrow (12.36\pm 0.005)+(14.13\pm 0.005)+(16.38\pm 0.005)=42.87\pm 0.015$

(iv) $12.36+14.13-16.38 \rightarrow (12.36\pm 0.005)+(14.13\pm 0.005)-(16.38\pm 0.005)=10.11\pm 0.015$

4. Find the relative error bound for each answer of Exercise 1.

A number a with absolute error bound ε_a has relative error bound $r_a \approx \varepsilon_a/|a|$. For the rounded numbers in Exercise 1, with absolute error bounds in Exercise 2,

(i) (a) $0.0005/1.213 = 0.0004$ (b) $0.0005/1.213 = 0.0004$

(ii) (a) $0.0005/72.030 = 0.000007$ (b) $0.005/72.03 = 0.00007$

(iii) (a) $0.0005/0.130 = 0.004$ (b) $0.00005/0.1299 = 0.0004$

(iv) (a) $0.0005/0.002 = 0.25$ (b) $0.0000005/0.0025 = 0.0002$

5. Compute the values of the following arithmetic expressions. Assuming that all the numbers in the expressions are correctly rounded, find the absolute error bounds of your answers:
(i) 22.7×2.59 , **(ii)** $22.7/2.59$, **(iii)** $(17.43-12.34)/14.38$

(i) The absolute and relative errors of the numbers are

$$a=22.7: \quad \varepsilon_a = 0.05, \quad r_a = 0.05/22.7 = 0.00220$$
$$b=2.59: \quad \varepsilon_b = 0.005, \quad r_b = 0.005/2.59 = 0.00193$$

Then $a\times b = 22.7\times 2.59 = 58.793$

$\to\ r_{a\times b} = r_a + r_b = 0.00220 + 0.00193 = 0.00413$

$\to\ \varepsilon_{a\times b} = r_{a\times b}\times(a\times b) = 0.00413\times 58.793 = 0.243$

Therefore $22.7\times 2.59 = 58.793 \pm 0.243$

(ii) $a\div b = 22.7\times 2.59 = 8.764$

$\to\ r_{a\div b} = r_{a\times b} = 0.00413$

$\to\ \varepsilon_{a\div b} = r_{a\div b}\times(a\div b) = 0.00413\times 8.764 = 0.2036$

Therefore $22.7\div 2.59 = 8.764 \pm 0.036$

(iii) Write $c/d = (17.43-12.34)/14.38$

We have $c = 17.43 - 12.34 = 5.09$

$\to\ \varepsilon_c = 0.005 + 0.005 = 0.01, \quad r_c = 0.01/5.09 = 0.00196$

and $d = 14.38 \ \to\ \varepsilon_d = 0.005, \quad r_d = 0.005/14.38 = 0.00035$

Then $c/d = 5.09/14.38 = 0.3540$

$\to\ r_{c/d} = r_c + r_d = 0.00196 + 0.00035 = 0.00231$

$\to\ \varepsilon_{c/d} = 0.00231\times 0.3540 = 0.0008$

Therefore $(17.43-12.34)/14.38 = 0.3540 \pm 0.0008$

6. Solve $x^2 - 60x + 1 = 0$ by **(i)** equations (20.3a) and **(ii)** equations (20.3b), using (a) 4-figure arithmetic, (b) 6-figure arithmetic.

We have $x^2 - 60x + 1 = 0 \quad \rightarrow \quad x = \frac{1}{2}(60 \pm \sqrt{3600 - 4}) = \frac{1}{2}(60 \pm 59.9667)$

(i) By equation (20.3a)

(a) $x_1 = \frac{1}{2}(60 + 59.97) = 60.0, \quad x_2 = \frac{1}{2}(60 - 59.97) = 0.015$

(b) $x_1 = \frac{1}{2}(60 + 59.9667) = 59.9835, \quad x_2 = \frac{1}{2}(60 - 59.9667) = 0.01665$

(ii) By equation (20.3b)

(a) $x_1 = \frac{1}{2}(60 + 59.97) = 60.0, \quad x_2 = 1/x_1 = 1/60.0 = 0.01667$

(b) $x_1 = \frac{1}{2}(60 + 59.9667) = 59.9835, \quad x_2 = 1/x_1 = 1/59.9835 = 0.0166713$

7. **(i)** Compute $f(x) = x(\sqrt{x+1} - \sqrt{x})$ on a 10-digit calculator (or similar) for

$$x = 1, 10^2, 10^4, 10^6, 10^8.$$

(ii) Show that the function can be written as $f(x) = \dfrac{x}{\sqrt{x+1} + \sqrt{x}}$.

Use this to recompute the function.

In Table 1:

(i) $f(x) = x(\sqrt{x+1} - \sqrt{x})$ on a 10-digit calculator.

(ii) $f(x) = x(\sqrt{x+1} - \sqrt{x}) \quad \rightarrow \quad \dfrac{x(\sqrt{x+1} - \sqrt{x})(\sqrt{x+1} + \sqrt{x})}{\sqrt{x+1} + \sqrt{x}} = \dfrac{x}{\sqrt{x+1} + \sqrt{x}}$

The alternative expression does not suffer from differencing errors; and

$$f(x) \rightarrow \sqrt{x}/2 \text{ as } x \rightarrow \infty$$

Table 1

x	**(i)**	**(ii)**
1	0.414213562	0.414213562
100	4.9875621	4.98756211
10000	49.9987	49.9987501
1000000	500	499.999875
100000000	4900	4999.99999

8. **(i)** Compute $\dfrac{e^x - e^{-x}}{2x} - 1$ on a 10-digit calculator (or similar) for $x = 1, 10^{-2}, 10^{-4}, 10^{-6}$.

(ii) Use the Taylor series to find an expression for the function that is accurate for small values of x.

(iii) Use this to recompute the function for $x = 10^{-2}, 10^{-4}, 10^{-6}$.

In Table 2:

(i) $\dfrac{e^x - e^{-x}}{2x} - 1$ on a 10-digit calculator

(ii)
$$\frac{e^x - e^{-x}}{2x} - 1 = \frac{1}{2x}\left[\left(1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \frac{x^5}{120} + \frac{x^6}{720} + \frac{x^7}{5040} + \cdots\right)\right.$$
$$\left. - \left(1 - x + \frac{x^2}{2} - \frac{x^3}{6} + \frac{x^4}{24} - \frac{x^5}{120} + \frac{x^6}{720} - \frac{x^7}{5040} + \cdots\right)\right] - 1$$
$$= \frac{1}{2x}\left[2x + \frac{x^3}{3} + \frac{x^5}{60} + \frac{x^7}{2520} + \cdots\right] - 1$$
$$\approx \frac{x^2}{6}\left[1 + \frac{x^2}{20} + \frac{x^4}{840}\right]$$

and $\dfrac{e^x - e^{-x}}{2x} - 1 \to \dfrac{x^2}{6}$ as $x \to 0$

(iii) $\dfrac{x^2}{6}\left[1 + \dfrac{x^2}{20} + \dfrac{x^4}{840}\right]$ on the 10-digit calculator

Table 2

x	**(i)**	**(ii)**
1	0.175201194	0.175198412
0.01	1.66585×10^{-5}	$1.666675000 \times 10^{-5}$
0.0001	5×10^{-8}	$1.666666668 \times 10^{-9}$
0.000001	0	$1.666666667 \times 10^{-13}$

Section 20.3

Find a solution to 4 significant figures of the following equations by the bisection method, using the given starting values of *x*:

9. $x^2 - \ln x = 2;\ x_< = 1.5,\ x_> = 1.6$

Write $f(x) = x^2 - \ln x - 2 = 0$. A root lies between $x_< = 1.5$ and $x_> = 1.6$, with $f(x_<) = -0.16 < 0$ and $f(x_>) = 0.09 > 0$. Then $x_3 = (x_< + x_>)/2 = 1.55$ and $f(x_3) = -0.036$, and the root lies between 1.55 and 1.6. The computation is summarized in the Table 3:

Table 3

n	$x_<;\quad f(x_<)$	$x_>;\quad f(x_>)$	$\frac{1}{2}(x_< + x_>);\ f$
0	1.5000; −0.1555	1.6000; +0.0900	1.5500; −0.0358
1	1.5500; −0.0358	1.6000; +0.0900	1.5750; +0.0264
2	1.5500; −0.0358	1.5750; +0.0264	1.5625; −0.0049
3	1.5625; −0.0049	1.5750; +0.0264	1.5688; +0.0108
4	1.5625; −0.0049	1.5688; +0.0108	1.5657; +0.0003
5	1.5625; −0.0049	1.5657; +0.0003	1.5641; −0.0009
6	1.5641; −0.0009	1.5657; +0.0003	1.5649; +0.0011
7	1.5641; −0.0009	1.5649; +0.0011	1.5645; +0.0001
8	1.5641; −0.0009	**1.5645**; +0.0001	**1.5643**; −0.0004

Therefore $1.5643 \le x \le 1.5645$ (to 4 significant figures)

10. $e^{-x} = \tan x$; 0.5, 0.6

Write $f(x) = e^{-x} - \tan x$. The computation is summarized in the Table 4:

Table 4

n	$x_<$; $f(x_<)$	$x_>$; $f(x_>)$	$\frac{1}{2}(x_< + x_>)$; f
0	0.60000; −0.13533	0.50000; +0.06023	0.55000; −0.03616
1	0.55000; −0.03616	0.50000; +0.06023	0.52500; +0.01234
2	0.55000; −0.03616	0.52500; +0.01234	0.53750; −0.01183
3	0.53750; −0.01183	0.52500; +0.01234	0.53125; +0.00027
4	0.53750; −0.01183	0.53125; +0.00027	0.53438; −0.00578
5	0.53438; −0.00578	0.53125; +0.00027	0.53282; −0.00276
6	0.53282; −0.00276	0.53125; +0.00027	0.53204; −0.00126
7	0.53204; −0.00126	0.53125; +0.00027	0.53165; −0.00050
8	0.53165; −0.00050	0.53125; +0.00027	0.53145; −0.00011
9	0.53145; −0.00011	0.53125; +0.00027	0.53135; +0.00008
10	0.53145; −0.00011	**0.53135**; +0.00008	**0.53140**; −0.00002

Therefore $0.53135 \le x \le 0.53140$ (to 4 significant figures)

11. $x^3 - 3x^2 + 6x = 5$; 1.0, 1.5

Write $f(x) = x^3 - 3x^2 + 6x - 5$. The computation is summarized in the Table 5:

Table 5

n	$x_<$; $f(x_<)$	$x_>$; $f(x_>)$	$\frac{1}{2}(x_< + x_>)$; f
0	1.00000; −1.00000	1.50000; +0.62500	1.25000; −0.23438
1	1.25000; −0.23438	1.50000; +0.62500	1.37500; +0.17773
2	1.25000; −0.23438	1.37500; +0.17773	1.31250; −0.03198
3	1.31250; −0.03198	1.37500; +0.17773	1.34375; +0.07187
4	1.31250; −0.03198	1.34375; +0.07187	1.32813; +0.02032
5	1.31250; −0.03198	1.32813; +0.02032	1.32032; −0.00617
6	1.32032; −0.00617	1.32813; +0.02032	1.32423; +0.00677
7	1.32032; −0.00617	1.32423; +0.00677	1.32228; +0.00031
8	1.32032; −0.00617	1.32228; +0.00031	1.32130; −0.00293
9	1.32130; −0.00293	1.32228; +0.00031	1.32179; −0.00131
10	1.32179; −0.00131	**1.32228**; +0.00031	**1.32204**; −0.00048

Therefore $1.32204 \le x \le 1.32228$

Find a solution to 8 significant figures of the following equations by the Newton–Raphson method starting in every case with $x_0 = 1$ (see Exercises 9 to 11):

12. $x^2 - \ln x = 2$

Write $f(x) = x^2 - \ln x - 2$. Then $f'(x) = 2x - 1/x$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^{\,2} - \ln x_n - 2}{2x_n - 1/x_n}$$

The calculation is summarized in Table 6:

Table 6

n	x_n	$f(x_n)/f'(x_n)$	x_{n+1}
0	1	−1	2
1	2	0.37338652	1.62661348
2	1.62661348	0.06040327	1.56621021
3	1.56621021	0.00174647	1.56446373
4	1.56446373	0.00000148	**1.56446226**
5	1.56446226	0.00000000	**1.56446226**

Therefore $x = 1.5644623$

13. $e^{-x} = \tan x$

Write $f(x) = e^{-x} - \tan x$. Then $f'(x) = -e^{-x} - \sec^2 x$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{e^{-x_n} - \tan x_n}{e^{-x_n} - \sec^2 x_n}$$

The calculation is summarized in Table 7:

Table 7

n	x_n	$f(x_n)/f'(x_n)$	x_{n+1}
0	1	0.313578539	0.686421461
1	0.686421461	0.145291364	0.541130097
2	0.541130097	0.009714010	0.531416087
3	0.531416087	0.000025230	**0.531390857**
4	0.531390857	0.000000000	**0.531390857**

Therefore $x = 0.53139086$

14. $x^3 - 3x^2 + 6x = 5$

Write $f(x) = x^3 - 3x^2 + 6x - 5$. Then $f'(x) = 3x^2 - 6x + 6$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^{\ 3} - 3x_n^{\ 2} + 6x_n - 5}{3x_n^{\ 2} - 6x_n + 6}$$

The calculation is summarized in Table 8:

Table 8

n	x_n	$f(x_n)/f'(x_n)$	x_{n+1}
0	1	−0.333333333	1.333333333
1	1.333333333	0.011111111	1.322222222
2	1.322222222	0.000036867	**1.322185355**
3	1.322185355	0.000000000	**1.322185355**

Therefore $x = 1.3221854$

15. Given one root, x_1, of a polynomial of degree *n*, a second root can be obtained by first dividing the polynomial by the factor $(x - x_1)$ to give a polynomial of degree $n-1$. Show that the computed root of the cubic in Exercises14 is the only real one.

The computed root of the cubic in Exercise 14 is $x = 1.322$ to 4 significant figures.
The cubic can then be written as

$$f(x) = x^3 - 3x^2 + 6x - 5 = (x - 1.322)(ax^2 + bx + c)$$

and the quadratic can be obtained by algebraic division (Section 2.6):

$$\begin{array}{r|l} & x^2 - 1.678x + 3.782 \\ \hline x - 1.322 & x^3 - 3x^2 \qquad + 6x - 5 \\ & \underline{x^3 - 1.322x^2} \\ & \quad -1.678x^2 + 6x \qquad - 5 \\ & \quad \underline{-1.678x^2 + 2.218x} \\ & \qquad\qquad 3.782x - 5 \\ & \qquad\qquad \underline{3.782x - 5} \\ & \qquad\qquad 0 \end{array}$$

The roots of the quadratic are

$$x^2 - 1.678x + 3.782 = 0 \text{ when } x = \frac{1}{2}\left[1.678 \pm \sqrt{1.678^2 - 4 \times 3.782}\right] = \frac{1}{2}\left[1.678 \pm \sqrt{-12.31}\right]$$

The discriminant is negative, so that the roots of the quadratic are complex, and the cubic has only the one real root.

Section 20.4

Six points on the graph of a function $y = f(x)$ are given by the (x, y) pairs

(0.0, 0.00000)	(0.2, 0.19867)	(0.4, 0.38942)
(0.6, 0.56464)	(0.8, 0.71736)	(1.0, 0.84147)

(the function is $\sin x$).

16. Use linear interpolation to compute $f(0.04)$, $f(0.26)$, $f(0.5)$, $f(0.81)$.

By equation (20.17)

$$y = y_0 + (x - x_0)\left(\frac{y_1 - y_0}{x_1 - x_0}\right)$$

(a) $y = f(0.04)$:

Use $(x_0, y_0) = (0.0, 0.0)$, $(x_1, y_1) = (0.2, 0.19867)$

Then $f(0.04) \approx 0.04 \times \dfrac{0.19867}{0.2} = 0.03973$

(b) $y = f(0.26)$:

Use $(x_0, y_0) = (0.2, 0.19867)$, $(x_1, y_1) = (0.4, 0.38942)$

Then $f(0.26) \approx 0.19867 + (0.26 - 0.2) \times \dfrac{0.38942 - 0.19867}{0.4 - 0.2} = 0.25590$

(c) $y = f(0.5)$:

Use $(x_0, y_0) = (0.4, 0.38942)$, $(x_1, y_1) = (0.6, 0.56464)$

Then $f(0.5) \approx 0.38942 + (0.5 - 0.4) \times \dfrac{0.56464 - 0.38942}{0.6 - 0.4} = 0.47703$

(d) $y = f(0.81)$:

Use $(x_0, y_0) = (0.8, 0.71736)$, $(x_1, y_1) = (1.0, 0.84147)$

Then $f(0.81) \approx 0.71736 + (0.81 - 0.8) \times \dfrac{0.84147 - 0.71736}{1.0 - 0.8} = 0.72357$

17. Use quadratic interpolation to compute $f(0.04),\ f(0.26),\ f(0.81)$.

By equation (20.18)

$$f(x) = L_0(x)y_0 + L_1(x)y_1 + L_2(x)y_2$$

where $$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)},\ L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)},\ L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

The calculations are summarized in Table 9.

(a) $y = f(0.04)$

Use $(x_0, y_0) = (0.0, 0.0),\ (x_1, y_1) = (0.2, 0.19867),\ (x_2, y_2) = (0.4, 0.38942)$

Then $f(0.04) \approx 0.4037$

(b) $y = f(0.26)$

Use $(x_0, y_0) = (0.0, 0.0),\ (x_1, y_1) = (0.2, 0.19867),\ (x_2, y_2) = (0.4, 0.38942)$

Then $f(0.26) \approx 0.25673$

(c) : $y = f(0.81)$

Use $(x_0, y_0) = (0.6, 0.56464),\ (x_1, y_1) = (0.8, 0.71736),\ (x_1, y_1) = (1.0, 0.84147)$

Then $f(0.81) \approx 0.72425$

Table 9

x	x_0	x_1	x_2	L_0	L_1	L_2	y_0	y_1	y_2	$f(x)$
0.04	0.0	0.2	0.4	0.72000	0.36000	−0.08000	0.00000	0.19867	0.38942	0.040368
0.26	0.0	0.2	0.4	−0.10500	0.91000	0.19500	0.00000	0.19867	0.38942	0.256727
0.81	0.6	0.8	1.0	−0.02375	0.99750	0.02625	0.56464	0.71736	0.84147	0.724245

18. Construct the finite difference interpolation table, and use it to compute $f(0.26)$.

By equations (20.19) to (20.23) the function can be approximated in terms of finite differences of the six points

$$(x_0, y_0) = (0.0, 0.00000),\quad (x_1, y_1) = (0.2, 0.19867),\quad (x_2, y_2) = (0.4, 0.38942),$$
$$(x_3, y_3) = (0.6, 0.56464),\quad (x_4, y_4) = (0.8, 0.71736),\quad (x_5, y_5) = (1.0, 0.84147)$$

by $f(x) = f(x_0) + (x - x_0)D_1 + (x - x_0)(x - x_1)D_2 + (x - x_0)(x - x_1)(x - x_2)D_3$
$$+(x - x_0)(x - x_1)(x - x_2)(x - x_3)D_4 + (x - x_0)(x - x_1)(x - x_2)(x - x_3)(x - x_4)D_5$$

where D_0 to D_5 are the finite differences defined by equations (20.19) and (20.20), and by Table 20.5. In the present case, they are given in Table 10.

Table 10

x	y	D_1	D_2	D_3	D_4	D_5
0	**0**					
		0.99335				
0.2	0.19867		**−0.09900**			
		0.95375		**−0.15855**		
0.4	0.38942		−0.19413		**0.01669**	
		0.87610		−0.14520		**0.00570**
0.6	0.56464		−0.28125		0.02239	
		0.76360		−0.12730		
0.8	0.71736		−0.35763			
		0.62055				
1.0	0.84147					

The formula gives a sequence of approximate values of the function. Thus, for $x = 0.26$, using the values of D_i in bold face in Table 10,

$$p_1(x) = f(x_0) + (x - x_0)D_1 \quad \rightarrow \quad f(0.26) \approx p_1(0.26) = 0.258271$$
$$p_2(x) = f(x_0) + (x - x_0)D_1 + (x - x_0)(x - x_1)D_2$$
$$= p_1(x) + (x - x_0)(x - x_1)D_2 \quad \rightarrow \quad f(0.26) \approx p_2(0.26) = 0.256727$$
$$p_3(x) = p_2(x) + (x - x_0)(x - x_1)(x - x_2)D_3 \quad \rightarrow \quad f(0.26) \approx p_3(0.26) = 0.257073$$
$$p_4(x) = p_3(x) + (x - x_0)(x - x_1)(x - x_2)(x - x_3)D_4 \quad \rightarrow \quad f(0.26) \approx p_4(0.26) = 0.257085$$
$$p_5(x) = p_4(x) + (x - x_0)(x - x_1)(x - x_2)(x - x_3)(x - x_4)D_5 \quad \rightarrow \quad f(0.26) \approx p_5(0.26) = 0.257083$$

The exact value (to 6 significant figures) is $\sin 0.26 = 0.257081$

Section 20.5

19. Find estimates of the integral

$$I = \int_{1.0}^{2.6} \frac{dx}{x}$$

by means of the trapezoidal rule (20.32) and the error formula (20.34), starting with one strip $(n = 1)$ and doubling the number of strips $(n = 2, 4, 8, \ldots)$ until 4-figure accuracy is obtained.

By equation (20.32),

$$I = \int_{1.0}^{2.6} \frac{dx}{x} \approx T(n) = h\left[\frac{1}{2} f_0 + f_1 + f_2 + \cdots + f_{n-1} + \frac{1}{2} f_n\right]$$

$$= h\sum_{i=0}^{n} T_i$$

where the quantities f_j are the values of the integrand $f(x) = 1/x$ at the $n+1$ points of the trapezoidal prescription, and $h = 1.6/n$ is the width of the interval. Table 11 shows the results for $n = 1, 2, 4, 8, 16$. For each value of *n*, the quantities listed are the contributions T_i of the points, the estimate $T(n)$ of the integral, the estimated error ε, from equation (20.34), and a corrected estimate of the integral. The exact value is $\ln 2.6 = 0.95551145$

Table 11

x_i	$f_i = 1/x_i$	$n = 1$	$n = 2$	$n = 4$	$n = 8$	$n = 16$
1.0	1	0.5	0.5	0.5	0.5	0.5
1.1	0.90909					0.909091
1.2	0.83333				0.83333	0.833333
1.3	0.76923					0.769231
1.4	0.71429			0.71429	0.71429	0.714286
1.5	0.66667					0.666667
1.6	0.625				0.625	0.625
1.7	0.58824				0	0.588235
1.8	0.55556		0.55556	0.55556	0.55556	0.555556
1.9	0.52632					0.526316
2.0	0.5				0.5	0.5
2.1	0.47619					0.47619
2.2	0.45455			0.45455	0.45455	0.454545
2.3	0.43478					0.434783
2.4	0.41667				0.41667	0.416667
2.5	0.4					0.4
2.6	0.38462	0.19231	0.19231	0.19231	0.19231	0.192308
	$T(n) =$	1.10769	0.99829	0.96668	0.95834	0.956221
	$\varepsilon =$	–0.18178	–0.04544	–0.01136	–0.00284	–0.000710
	$T(n) + \varepsilon =$	0.92592	0.95285	0.95532	**0.95550**	**0.955511**

20. Use Simpson's rule (20.35) for $2n = 2, 4, 8, \ldots$ to find the value of the integral $I = \int_{1.0}^{2.6} \frac{dx}{x}$ to 4 decimal places

By equation (20.35),

$$I(h) = \int_{1.0}^{2.6} \frac{dx}{x} \approx S(2n) = \frac{h}{3}\Big[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{2n-1} + f_{2n} \Big]$$

$$= \frac{h}{3}\sum_{i=0}^{2n} S_i$$

where the quantities f_j are the values of the integrand $f(x) = 1/x$ at the $2n+1$ points of the Simpson prescription, and $h = 1.6/2n$ is the width of the interval. Table 12 shows the results for $n = 1, 2, 4, 8$. For each value of *n*, the quantities listed are the contributions S_i of the points and the estimate $S(2n)$ of the integral.

Table 12

x_i	$f_i = 1/x_i$	$2n = 2$	$2n = 4$	$2n = 8$	$2n = 16$
1.0	1.00000000	1.00000000	1.00000000	1.00000000	1.00000000
1.1	0.90909091				3.63636364
1.2	0.83333333			3.33333333	1.66666667
1.3	0.76923077				3.07692308
1.4	0.71428571		2.85714286	1.42857143	1.42857143
1.5	0.66666667				2.66666667
1.6	0.62500000			2.50000000	1.25000000
1.7	0.58823529				2.35294118
1.8	0.55555556	2.22222222	1.11111111	1.11111111	1.11111111
1.9	0.52631579				2.10526316
2.0	0.50000000			2.00000000	1.00000000
2.1	0.47619048				1.90476190
2.2	0.45454545		1.81818182	0.90909091	0.90909091
2.3	0.43478261				1.73913043
2.4	0.41666667			1.66666667	0.83333333
2.5	0.40000000				1.60000000
2.6	0.38461538	0.38461538	0.38461538	0.38461538	0.38461538
	$S(2n) =$	0.95614016	0.95614016	**0.95555926**	**0.95551463**

21. (i) The error in Simpson's rule is Ah^4 when h is small enough, and A is a constant. If $S(2n)$ is the Simpson formula for $2n$ intervals, show that

$$I = \int_a^b f(x)\,dx \approx \frac{1}{15}[16S(2n) - S(n)] \qquad \text{(Richardson's extrapolation).}$$

(ii) Use this and the results of Exercise 20 to estimate a more accurate value of the integral.

(i) If $I(h) \approx S(n) + Ah^4$

then $I(h/2) \approx S(2n) + A(h/2)^4 \;\rightarrow\; 16I(h/2) \approx 16S(2n) + Ah^4$

Therefore, if $I(h/2) \approx I(h)$ then $I \approx \frac{1}{15}[16S(2n) - S(n)]$

(ii) By Richardson's extrapolation and the results in Exercise 20 for $S(16)$ and $S(8)$

$$\int_{1.0}^{2.6} \frac{dx}{x} \approx \frac{1}{15}[16S(16) - S(8)] = \frac{1}{15}[16\times 0.95551463 - 0.95555926\,]$$

$$= 0.95551165 \qquad \text{(exact: } 0.5551145)$$

Use Simpson's rule for $2n = 2, 4, 8, \ldots$ to find the values of the following integrals to 5 decimal places:

22. $\int_0^1 \frac{\sin x}{x}\,dx$: As Exercise 20, with Richardson's extrapolation.

Table 13

x_i	$f_i = \sin x_i / x_i$	$2n = 2$	$2n = 4$	$2n = 8$	$2n = 16$
0	1	1.00000000	1.00000000	1.00000000	1.00000000
0.0625	0.99934909				3.99739634
0.1250	0.99739787			3.98959147	1.99479573
0.1875	0.99415092				3.97660366
0.2500	0.98961584		3.95846335	1.97923167	1.97923167
0.3125	0.98380325				3.93521299
0.3750	0.97672674			3.90690698	1.95345349
0.4375	0.96840287				3.87361149
0.5000	0.95885108	3.83540431	1.91770215	1.91770215	1.91770215
0.5625	0.94809364				3.79237457
0.6250	0.93615564			3.74462255	1.87231127
0.6875	0.92306484				3.69225937
0.7500	0.90885168		3.63540672	1.81770336	1.81770336
0.8125	0.89354911				3.57419646
0.8750	0.87719257			3.50877030	1.75438515
0.9375	0.85981985				3.43927940
1	0.84147098	0.38461538	0.84147098	0.84147098	0.84147098
$S(2n)$		0.94614588	0.98393041	0.94608331	**0.94608309**
$\frac{1}{15}[16S(2n) - S(n)]$			0.98644938	0.94356017	**0.94608307**

The computed value of the integral, with $2n = 16$ and Richardson's extrapolation, is identical to the exact value 0.94608307 to 8 decimal places.

23. $\int_0^2 e^{-x^2}\,dx$: As Exercise 20, with Richardson's extrapolation.

Table 14

x_i	$f_i = \exp(-x_i^2)$	$2n=2$	$2n=4$	$2n=8$	$2n=16$
0	1.00000000	1.00000000	1.00000000	1.00000000	1.00000000
0.125	0.98449644				3.93798575
0.250	0.93941306			3.75765225	1.87882613
0.375	0.86881506				3.47526023
0.500	0.77880078		3.11520313	1.55760157	1.55760157
0.625	0.67663385				2.70653538
0.750	0.56978282			2.27913130	1.13956565
0.875	0.46504319				1.86017275
0	0.36787944	1.47151776	0.73575888	0.73575888	0.73575888
1.125	0.28206295				1.12825181
1.250	0.20961139			0.83844555	0.41922277
1.375	0.15097742				0.60390967
1.500	0.10539922		0.42159690	0.21079845	0.21079845
1.625	0.07131668				0.28526673
1.750	0.04677062			0.18708249	0.09354124
1.875	0.02972922				0.11891687
2	0.01831564	0.01831564	0.01831564	0.01831564	0.01831564
$S(2n)$		0.82994447	0.88181243	0.88206551	**0.88208040**
$\frac{1}{15}[16S(2n)-S(n)]$			0.88527029	0.88208238	**0.88208139**

The computed value of the integral, with $2n=16$ and Richardson's extrapolation, is identical to the exact value 0.88208139 to 8 decimal places.

24. **(i)** Use the Euler-MacLaurin formula to calculate the sum $S(11)=\sum_{m=0}^{\infty} 1\big/(11+m)^2$ to six decimal places. **(ii)** Use the value of $S(10)$ in Example 20.12 to verify that $S(11)=S(10)-0.01$.

In Example 20.12,

$$S(a)=\sum_{m=0}^{\infty}\frac{1}{(a+m)^2}=\frac{1}{a}+\frac{1}{2a^2}+\frac{1}{6a^3}-\frac{1}{30^5}+\frac{1}{42a^7}-\cdots$$

(i)

$$S(11)=\sum_{m=0}^{\infty}\frac{1}{(11+m)^2}=\frac{1}{11}+\frac{1}{2\times(11)^2}+\frac{1}{6\times(11)^3}-\frac{1}{30\times(11)^5}+\frac{1}{42\times(11)^7}-\cdots$$

$$=0.09090909+0.00413223+0.00012522-0.00000021+\cdots$$

$$\approx 0.09516633$$

(ii) Now, by by Example 20.12, $S(10)\approx 0.105166$. Therefore

$$\sum_{m=0}^{\infty}\frac{1}{(11+m)^2}=\frac{1}{11}+\frac{1}{(11)^2}+\frac{1}{(11)^3}+\cdots=\sum_{m=0}^{\infty}\frac{1}{(10+m)^2}-\frac{1}{(10)^2}$$

$$\to\quad S(11)=S(10)-0.01\approx 0.105166-0.01$$

$$\approx 0.095166$$

25. Use the results of Exercise 24 to **c**alculate $S(1)$ to six significant figures.

(i) We have $$\sum_{m=0}^{\infty}\frac{1}{(1+m)^2}=\sum_{m=0}^{9}\frac{1}{(1+m)^2}+\sum_{m=10}^{\infty}\frac{1}{(1+m)^2}$$
$$=\sum_{m=0}^{9}\frac{1}{(1+m)^2}+\sum_{m=0}^{\infty}\frac{1}{(11+m)^2}$$

Therefore $$S(1)=\sum_{m=0}^{9}\frac{1}{(1+m)^2}+S(11)\approx 1.54976773+0.09516333\approx 1.64493$$

26. Calculate $\ln 1!$, $\ln 2!$ and $\ln 3!$ **(i)** using the "large-number" formula $n\ln n-n$, **(ii)** from the more accurate formula given in Example 20.14. **(iii)** Exactly.

We have **(i)** $\ln n!\approx n\ln n-n$

(ii) $\ln n!\approx n\ln n-n+\dfrac{1}{2}\ln 2\pi n+\dfrac{1}{12n}-\dfrac{1}{360n^3}+\dfrac{1}{1260n^5}$

(iii) $\ln n!=\ln(1\times 2\times\cdots\times n)$

Table 15

n	**(i)**	**(ii)**	**(iii)**
1	−1	0.0003	0
2	−0.6137	0.693151	0.693147
3	0.2958	1.7917597	1.7917595

Section 20.7

Solve the following systems of equations by the Gauss elimination method:

27. (1) $x_1-4x_2=-2$
(2) $3x_1+x_2=7$

1. Elimination of x_1

Choose equation (1) as the pivot equation, and eliminate x_1 from the second equation by subtracting 3 × equation (1) from equation (2) to give

(1) $x_1-4x_2=-2$
(2′) $13x_2=13$

2. Back substitution; the equations are solved in reverse order:

(2′) $13x_2=13\ \rightarrow\ x_2=1$
(1) $x_1-4x_2=-2\ \rightarrow\ x_1=2$

28.
$$\begin{array}{ll} (1) & 2x_1 + x_2 - x_3 = 6 \\ (2) & 4x_1 \quad\;\; - x_3 = 6 \\ (3) & 8x_1 + 2x_2 + 2x_3 = -8 \end{array}$$

1. Elimination of x_1 from equations (2) and (3), and of x_2 from (3):

$$\begin{array}{rcll} & & (1) & 2x_1 + x_2 - x_3 = 6 \\ (2)-2\times(1) & \to & (2') & -2x_2 + x_3 = -6 \\ (3)+4\times(1)+3\times(2') & \to & (3') & x_3 = -2 \end{array}$$

2. Back substitution:

$$(3')\ x_3 = -2 \ \to\ (2')\ x_2 = 2 \ \to\ (1)\ x_1 = 1$$

Therefore $x_1 = 1, x_2 = 2, x_3 = -2$

29.
$$\begin{array}{ll} (1) & x + y + z = 2 \\ (2) & -x + 2y - 3z = 32 \\ (3) & 3x \quad\;\; - 4z = 17 \end{array}$$

1. Elimination of x from equations (2) and (3) and of y from equation (3):

$$\begin{array}{rcll} & & (1) & x + y + z = 2 \\ (2)+(1) & \to & (2') & 3y - 2z = 34 \\ (3)-3\times(1)+(2') & \to & (3') & -9z = 45 \end{array}$$

2. Back substitution:

$$(3'')\ z = -5 \ \to\ (2')\ y = 8 \ \to\ (1)\ x = -1$$

Therefore $x = -1,\ y - 8,\ z = -5$

30.
$$\begin{array}{ll} (1) & w + 2x + 3y + z = 5 \\ (2) & 2w + x + y + z = 3 \\ (3) & w + 2x + y \quad\; = 4 \\ (4) & \quad\;\; x + y + 2z = 0 \end{array}$$

1. Elimination of w from equations (2) and (3), and of x and y from equation (4):

$$\begin{array}{rcll} & & (1) & w + 2x + 3y + z = 5 \\ (2)-2\times(1) & \to & (2') & -3x - 5y - z = -7 \\ (3)-(1) & \to & (3') & -2y - z = -1 \\ 3\times(4)+(2')-(3') & \to & (4') & 6z = -6 \end{array}$$

2. Back substitution:

$$(4')\ z = -1 \ \to\ (3')\ y = 1 \ \to\ (2')\ x = 1 \ \to\ (1)\ w = 1$$

Therefore $w = x = y = 1,\ z = -1$

31. **(i)** Use Gauss elimination to find the value of λ for which the following equations have a solution.

(ii) Solve the equations for this value of λ:

$$\begin{array}{ll} (1) & x + y + z = 2 \\ (2) & -x + 2y - 3z = 32 \\ (3) & 3x \quad + 5z = \lambda \end{array}$$

(i) Elimination of x from equations (2) and (3) and of y from equation (3):

$$\begin{array}{rcll} & & (1) & x + y + z = 2 \\ (2)+(1) & \to & (2') & 3y - 2z = 34 \\ (3)-3\times(1)+(2') & \to & (3') & = \lambda + 28 \end{array}$$

The equations are consistent when $\lambda = -28$.

(ii) The equations are linearly dependent for this value of λ; thus $(3) = 2\times(1)-(2)$. We can use equations $(2')$ and (3) to solve for x and y in terms of (arbitrary) z. Then

$$\begin{array}{lll} (2') & 3y - 2z = 34 & \to\; y = \frac{1}{3}(34+2z) \\ (3) & 3x + 5z = -28 & \to\; x = -\frac{1}{3}(28+5z) \end{array}$$

Section 20.8

32. Use Gauss–Jordan elimination to find the inverse of the matrix

$$\mathbf{A} = \begin{pmatrix} -1 & 1 & 2 \\ 3 & -1 & 1 \\ -1 & 3 & 4 \end{pmatrix}$$

We follow the procedure described in Example 20.17.

(a) The augmented matrix of the problem is

$$(\mathbf{A}|\mathbf{I}) = \left(\begin{array}{rrr|rrr} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right)$$

(b) The matrix **A** is reduced to upper triangular form by Gauss elimination:

$$\begin{array}{l} \\ \text{row: } (2)+3\times(1) \\ \text{row: } (3)-(1) \end{array} \to \left(\begin{array}{rrr|rrr} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 7 & 3 & 1 & 0 \\ 0 & 2 & 2 & -1 & 0 & 1 \end{array}\right)$$

$$\begin{array}{l} \\ \\ \text{row: } (3)-(2) \end{array} \to \left(\begin{array}{rrr|rrr} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 7 & 3 & 1 & 0 \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right)$$

(c) It is reduced to diagonal form by further elimination steps:

$$\begin{array}{l} \text{row }(1)+2/5\times(3) \\ \text{row }(2)+7/5\times(3) \end{array} \quad \to \left(\begin{array}{ccc|ccc} -1 & 1 & 0 & -3/5 & -2/5 & 2/5 \\ 0 & 2 & 0 & -13/5 & -2/5 & 7/5 \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right)$$

$$\begin{array}{l} \text{row }(1)+2/5\times(3) \\ \text{row }(2)+7/5\times(3) \end{array} \quad \to \left(\begin{array}{ccc|ccc} -1 & 1 & 0 & -3/5 & -2/5 & 2/5 \\ 0 & 2 & 0 & -13/5 & -2/5 & 7/5 \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right)$$

$$\text{row }(1)-(1/2)\times(2) \quad \to \left(\begin{array}{ccc|ccc} -1 & 0 & 0 & 7/10 & -2/10 & -3/10 \\ 0 & 2 & 0 & -13/5 & -2/5 & 7/5 \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right)$$

(d) It is reduced to the unit matrix by dividing by the diagonal element in each row:

$$\begin{array}{l} \text{row }(1)\div(-1) \\ \text{row }(2)\div(2) \\ \text{row }(1)\div(-5) \end{array} \quad \to \left(\begin{array}{ccc|ccc} 1 & 0 & 0 & -7/10 & 2/10 & 3/10 \\ 0 & 1 & 0 & -13/10 & -2/10 & 7/10 \\ 0 & 0 & 1 & 4/5 & 1/5 & -1/5 \end{array}\right)$$

The right half of the augmented matrix is the inverse matrix $\mathbf{A}^{-1}$:

$$\mathbf{A}^{-1} = \frac{1}{10}\begin{pmatrix} -7 & 2 & 3 \\ -13 & -2 & 7 \\ 8 & 2 & -2 \end{pmatrix}$$

Thus $$\mathbf{A}^{-1}\mathbf{A} = \frac{1}{10}\begin{pmatrix} -7 & 2 & 3 \\ -13 & -2 & 7 \\ 8 & 2 & -2 \end{pmatrix}\begin{pmatrix} -1 & 1 & 2 \\ 3 & -1 & 1 \\ -1 & 3 & 4 \end{pmatrix} = \frac{1}{10}\begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 10 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

33. Given the system of equations,

$$\begin{aligned} -x - y + 2z &= b_1 \\ 3x - y + z &= b_2 \\ -x + 3y + 4z &= b_3 \end{aligned}$$

use the result of Exercise 32 to express *x*, *y*, and *z* in terms of the arbitrary numbers b_1, b_2 and b_3.

The equations correspond to the matrix equation

$$\mathbf{Ax} = \mathbf{b} \quad \to \quad \begin{pmatrix} -1 & 1 & 2 \\ 3 & -1 & 1 \\ -1 & 3 & 4 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

Then, $$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \quad \to \quad \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{1}{10}\begin{pmatrix} -7 & 2 & 3 \\ -13 & -2 & 7 \\ 8 & 2 & -2 \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \quad \to \quad \begin{cases} x = \frac{1}{10}(-7b_1 + 2b_2 + 3b_3) \\ y = \frac{1}{10}(-13b_1 - 2b_2 + 7b_3) \\ z = \frac{1}{10}(8b_1 + 2b_2 - 2b_3) \end{cases}$$

Section 20.9

NOTE: The arithmetic for the following exercises is tedious. You are advised to use a spreadsheet or write your own computer programs to perform the tasks.

34. Apply Euler's method to the initial value problem

$$y'(x) = -y(x), \qquad y(0) = 1$$

with step sizes **(i)** $h = 0.2$, **(ii)** $h = 0.1$, **(iii)** $h = 0.05$ to calculate approximate values of $y(x)$ for $x = 0.2, 0.4, 0.6, 0.8, 1.0$. Compare these with the values obtained from the exact solution $y = e^{-x}$.

We have $f(x_n, y_n) = y'(x_n)$ in equation (20.54). Therefore

$$y_{n+1} = y_n + hy'(x_n) = y_n - hy_n$$

The results of applying the Euler recursion relation are summarized in Table 16.

Table		**(i)** $h = 0.2$		**(ii)** $h = 0.1$		**(iii)** $h = 0.05$	
x	$\exp(-x)$	y	error	y	error	y	error
0.00	1.000000	1.000000	0.000000	1.000000	0.000000	1.000000	0.000000
0.05	0.951229					0.950000	–0.001229
0.10	0.904837			0.900000	–0.004837	0.902500	–0.002337
0.15	0.860708					0.857375	–0.003333
0.20	0.818731	0.800000	–0.018731	0.810000	–0.008731	0.814506	–0.004225
0.25	0.778801					0.773781	–0.005020
0.30	0.740818			0.729000	–0.011818	0.735092	–0.005726
0.35	0.704688					0.698337	–0.006351
0.40	0.670320	0.640000	–0.030320	0.656100	–0.014220	0.663420	–0.006900
0.45	0.637628					0.630249	–0.007379
0.50	0.606531			0.590490	–0.016041	0.598737	–0.007794
0.55	0.576950					0.568800	–0.008150
0.60	0.548812	0.512000	–0.036812	0.531441	–0.017371	0.540360	–0.008452
0.65	0.522046					0.513342	–0.008704
0.70	0.496585			0.478297	–0.034856	0.487675	–0.008910
0.75	0.472367					0.463291	–0.009075
0.80	0.449329	0.409600	–0.039729	0.430467	–0.018862	0.440127	–0.009202
0.85	0.427415					0.418120	–0.009295
0.90	0.406570			0.387420	–0.019149	0.397214	–0.009355
0.95	0.386741					0.377354	–0.009387
1.00	0.367879	**0.327680**	**–0.040199**	**0.348678**	**–0.019201**	**0.358486**	**–0.009394**

The values and errors of $y(1.0)$ are (i) 0.327680 and –0.040199 for $h = 0.2$, (ii) 0.348678 and –0.019201 for $h = 0.1$, (iii) 0.358486 and –0.009394 for $h = 0.05$, compared to the exact value $e^{-1} = 0.367879$.

For initial value problems in Exercises 35 to 37, **(i)** apply Euler's method with step size $h = 0.1$ to compute an approximate value of $y(1)$, **(ii)** confirm the given exact solution and compute the error:

35. $y' = 2 - 2y, \quad y(0) = 0; \quad y = 1 - e^{-2x}$

(i) The Euler recursion relation is

$$y_{n+1} = y_n + h(2 - 2y_n)$$

and the results are summarized in Table 17.

(ii) If $y = 1 - e^{-2x}$ then $y' = 2e^{-2x} = 2 - 2y$, as required.

Then: exact value: $y(1) = 1 - e^{-2} = 0.864665$

approximate: $y(1) \approx y_{10} = 0.892626$

error: $\varepsilon_{10} = y_{10} - y(1) = 0.027961$

36. $y' = \dfrac{y^2}{x+1}, \quad y(0) = 1; \quad y = \dfrac{1}{1 - \ln(x+1)}$

(i) The Euler recursion relation is

$$y_{n+1} = y_n + h\frac{y_n^{\,2}}{x_n + 1}$$

and the results are summarized in Table 18.

(ii) If $y = \dfrac{1}{1 - \ln(x+1)}$ then $y' = \dfrac{-1}{(1 - \ln(x+1))^2} \times \dfrac{-1}{x+1} = \dfrac{y^2}{x+1}$.

Then: exact value: $y(1) = 1/(1 - \ln 2) = 3.258891$

approximate: $y(1) \approx y_{10} = 2.845387$

error: $\varepsilon_{10} = y_{10} - y(1) = -0.4135041$

Table 17	x_n	y_n
$n = 0$	0.00	0.000000
1	0.10	0.200000
2	0.20	0.360000
3	0.30	0.488000
4	0.40	0.590400
5	0.50	0.672320
6	0.60	0.737856
7	0.70	0.790285
8	0.80	0.832228
9	0.90	0.865782
10	1.00	**0.892626**

Table 18	x_n	y_n
$n = 0$	0.00	1.000000
1	0.10	1.100000
2	0.20	1.210000
3	0.30	1.332008
4	0.40	1.468489
5	0.50	1.622522
6	0.60	1.798027
7	0.70	2.000083
8	0.80	2.235397
9	0.90	2.513008
10	1.00	**2.845387**

37. $y' = \dfrac{y + x^2 - 2}{x+1}$, $y(0) = 2$; $y = x^2 + 2x + 2 - 2(x+1)\ln(x+1)$

(i) The Euler recursion relation is

$$y_{n+1} = y_n + h\left(\frac{y_n + x_n^{\;2} - 2}{x_n + 1}\right)$$

and the results are summarized in Table 19.

(ii) If $y = x^2 + 2x + 2 - 2(x+1)\ln(x+1)$ then $y' = 2x - 2\ln(x+1) = \dfrac{y + x^2 - 2}{x+1}$

Then: exact value: $y(1) = 5 - 4\ln 2 = 2.227411$

approximate: $y(1) \approx y_{10} = 2.191160$

error: $\varepsilon_{10} = y_{10} - y(1) = -0.036251$

Table 19	x_n	y_n
$n = 0$	0.00	2.000000
1	0.10	2.000000
2	0.20	2.000909
3	0.30	2.004318
4	0.40	2.011573
5	0.50	2.023829
6	0.60	2.042084
7	0.70	2.067214
8	0.80	2.099991
9	0.90	2.141102
10	1.00	**2.191160**

38. Apply the second-order Runge–Kutta method to the initial value problem in Exercise 34 with step sizes **(i)** $h = 0.2$, **(ii)** $h = 0.1$.

We have $y'(x) = -y(x), \quad y(0) = 1$

By equations (20.55),

$$y_{n+1} = y_n + hk_2$$

where k_2 is an estimate of the slope midway between x_n and x_{n+1} ,

$$k_2 = f(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_1) = y'(x_n + h/2)$$

and $k_1 = f(x_n, y_n) = y'(x_n)$

is the slope at point *n*. The results of the calculation are summarized in Tables 20 and 21.

(i) Table 20. $h = 0.2$

x	k_1	k_2	y	exact	error
0	−1.00000	−0.90000	1.000000	1.000000	0.000000
0.2	−0.82000	−0.73800	0.820000	0.818731	0.001269
0.4	−0.67240	−0.60516	0.672400	0.670320	0.002080
0.6	−0.55136	−0.49623	0.551368	0.548812	0.002556
0.8	−0.45212	−0.40691	0.452122	0.449329	0.002793
1	−0.37074	−0.33366	**0.370740**	0.367879	**0.002860**

(ii) Table 21 $h = 0.1$

x	k_1	k_2	y	exact	error
0	−1.000000	−0.950000	1.000000	1.000000	0.000000
0.1	−0.905000	−0.859750	0.905000	0.904837	0.000163
0.2	−0.819025	−0.778074	0.819025	0.818731	0.000294
0.3	−0.741218	−0.704157	0.741218	0.740818	0.000399
0.4	−0.670802	−0.637262	0.670802	0.670320	0.000482
0.5	−0.607076	−0.576722	0.607076	0.606531	0.000545
0.6	−0.549404	−0.521933	0.549404	0.548812	0.000592
0.7	−0.497210	−0.472350	0.497210	0.496585	0.000625
0.8	−0.449975	−0.427476	0.449975	0.449329	0.000646
0.9	−0.407228	−0.386866	0.407228	0.406570	0.000658
1	−0.368541	−0.350114	**0.368541**	0.367879	**0.000662**

The values of $y(1.0)$ are **(i)** 0.370740 for $h = 0.2$, **(ii)** 0.368541for $h = 0.1$, compared to the exact value $e^{-1} = 0.367879$ (compare Exercise 34).

39. Apply the fourth-order Runge–Kutta method to the initial value problem in Exercise 34 with step sizes **(i)** $h = 0.2$, **(ii)** $h = 0.1$.

We have $y'(x) = -y(x), \quad y(0) = 1$

The prescription for the fourth-order Runge-Kutta method is given by equations (20.56). The results of the calculation are summarized in Tables 22 and 23.

(i) Table 22. $h = 0.2$

x	k_1	k_2	k_3	k_4	y	exact	error
0	−1.00000	−0.90000	−0.91000	−0.81800	1.00000000	1.00000000	0.00000000
0.2	−0.81873	−0.73686	−0.74504	−0.66972	0.81873333	0.81873075	0.00000258
0.4	−0.67032	−0.60329	−0.60999	−0.54832	0.67032427	0.67032005	0.00000423
0.6	−0.54881	−0.49393	−0.49942	−0.44893	0.54881682	0.54881164	0.00000519
0.8	−0.44933	−0.40440	−0.40889	−0.36755	0.44933463	0.44932896	0.00000566
1	−0.36788	−0.33109	−0.33477	−0.30093	**0.36788524**	0.36787944	**0.00000580**

(ii) Table 23. $h = 0.1$

x	k_1	k_2	k_3	k_4	y	exact	error
0	−1.00000	−0.95000	−0.95250	−0.90475	1.00000000	1.00000000	0.00000000
0.1	−0.90483	−0.85959	−0.86185	−0.81865	0.90483750	0.90483742	0.00000008
0.2	−0.81873	−0.77779	−0.77984	−0.74074	0.81873090	0.81873075	0.00000015
0.3	−0.74081	−0.70377	−0.70563	−0.67025	0.74081842	0.74081822	0.00000020
0.4	−0.67032	−0.63680	−0.63848	−0.60647	0.67032029	0.67032005	0.00000024
0.5	−0.60653	−0.57620	−0.57772	−0.54875	0.60653093	0.60653066	0.00000027
0.6	−0.54881	−0.52137	−0.52274	−0.49653	0.54881193	0.54881164	0.00000030
0.7	−0.49658	−0.47175	−0.47299	−0.44928	0.49658562	0.49658530	0.00000031
0.8	−0.44932	−0.42686	−0.42798	−0.40653	0.44932929	0.44932896	0.00000033
0.9	−0.40657	−0.38624	−0.38725	−0.36784	0.40656999	0.40656966	0.00000033
1	−0.36788	−0.34948	−0.35040	−0.33283	**0.36787977**	0.36787944	**0.00000033**

The values of $y(1.0)$ are **(i)** 0.36788524 for $h = 0.2$,

(ii) 0.36787977 for $h = 0.1$,

compared to the exact value $e^{-1} = 0.36787944$ (compare Exercises 34 and 38).

Apply the fourth-order Runge–Kutta method to the initial value problems in Exercises 35, 36, and 37 with step size $h = 0.1$ to compute **(i)** $y(1)$ and **(ii)** the error:

The prescription for the fourth-order Runge-Kutta method is given by equations (20.56).

40. As Exercise 35

We have $y' = 2 - 2y, \quad y(0) = 0; \quad y = 1 - e^{-2x}$

Table 24. $h = 0.1$

x	k_1	k_2	k_3	k_4	y	exact	error
0	2.000000	1.800000	1.820000	1.636000	0.00000000	0.00000000	0.00000000
0.1	1.637467	1.473720	1.490095	1.339448	0.18126667	0.18126925	–0.00000258
0.2	1.340649	1.206584	1.219990	1.096651	0.32967573	0.32967995	–0.00000423
0.3	1.097634	0.987870	0.998847	0.897864	0.45118318	0.45118836	–0.00000519
0.4	0.898669	0.808802	0.817789	0.735111	0.55066537	0.55067104	–0.00000566
0.5	0.735770	0.662193	0.669551	0.601860	0.63211476	0.63212056	–0.00000580
0.6	0.602400	0.542160	0.548184	0.492763	0.69880009	0.69880579	–0.00000570
0.7	0.493205	0.443884	0.448816	0.403442	0.75339760	0.75340304	–0.00000544
0.8	0.403803	0.363423	0.367461	0.330311	0.79809839	0.79810348	–0.00000509
0.9	0.330607	0.297546	0.300853	0.270437	0.83469642	0.83470111	–0.00000469
1	0.270679	0.243611	0.246318	0.221416	**0.86466045**	0.86466472	**–0.00000427**

41. As Exercise 36

We have $y' = \frac{y^2}{x+1}, \quad y(0) = 1; \quad y = \frac{1}{1 - \ln(x+1)}$

Table 25. $h = 0.1$

x	k_1	k_2	k_3	k_4	y	exact	error
0	1.000000	1.050000	1.055006	1.111029	1.00000000	1.00000000	0.00000000
0.1	1.110727	1.171877	1.178058	1.246760	1.10535068	1.10535122	–0.00000055
0.2	1.246386	1.321582	1.329325	1.414216	1.22297331	1.22297464	–0.00000133
0.3	1.413745	1.507055	1.516930	1.622981	1.35568023	1.35568269	–0.00000246
0.4	1.622376	1.739595	1.752458	1.886840	1.50709184	1.50709594	–0.00000410
0.5	1.886039	2.035600	2.052775	2.226089	1.68198054	1.68198707	–0.00000653
0.6	2.224998	2.419505	2.443116	2.671539	1.88679518	1.88680537	–0.00001020
0.7	2.669997	2.928947	2.962543	3.271720	2.13049152	2.13050743	–0.00001592
0.8	3.269448	3.624252	3.674082	4.106625	2.42590312	2.42592831	–0.00002519
0.9	4.103110	4.606991	4.684767	5.315731	2.79211547	2.79215650	–0.00004103
1	5.309958	6.058940	6.188387	7.160118	**3.25882141**	3.25889135	**–0.0000699**

42. As Exercise 37

We have $y' = \dfrac{y + x^2 - 2}{x+1}$, $y(0) = 2$; $y = x^2 + 2x + 2 - 2(x+1)\ln(x+1)$

Table 26. $h = 0.1$

x	k_1	k_2	k_3	k_4	y	exact	error
0	0.000000	0.002381	0.002494	0.009318	2.00000000	2.00000000	0.00000000
0.1	0.009380	0.020249	0.020722	0.035325	2.00031780	2.00031760	0.00000020
0.2	0.035357	0.053357	0.054077	0.075259	2.00242860	2.00242826	0.00000033
0.3	0.075272	0.099346	0.100238	0.127055	2.00785334	2.00785291	0.00000043
0.4	0.127056	0.156366	0.157377	0.189077	2.01787823	2.01787774	0.00000049
0.5	0.189070	0.222941	0.224034	0.260005	2.03360522	2.03360468	0.00000055
0.6	0.259993	0.297872	0.299020	0.338759	2.05598898	2.05598839	0.00000059
0.7	0.338744	0.380172	0.381356	0.424445	2.08586457	2.08586395	0.00000063
0.8	0.424427	0.469022	0.470227	0.516311	2.12396866	2.12396801	0.00000066
0.9	0.516293	0.563728	0.564945	0.613725	2.17095592	2.17095523	0.00000069
1	0.613706	0.663706	0.664926	0.716145	**2.22741199**	2.22741128	**0.00000071**